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Surface relief influence on rheed oscillations shape during MBE growth

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Molecular beam epitaxy (MBE) is one of the basic methods for low-dimensional structures production. RHEED intensity oscillations being widely practiced as the method of growing surface control allow to determine thickness of the obtained film with an accuracy of one monolayer. However, oscillations damping with time and distortions of their shapes decrease the accuracy of thickness determination. Surface relief have a great impact on electronic properties of grown structures. But it's a cumbersome task to combine MBE technology with the direct observation of the surface during the growth process. Complicated shape of oscillations contains information not only on the number of growing monolayers but on the initial microrelief, evolution of this relief through the surface processes and the final morphology of grown layer. Relationship between RHEED oscillations shapes and microrelief of growing film is demonstrated.

Simulation of MBE growth process was carried out by Monte Carlo method in assumption of the SOS deposition on the Kossel crystal (100) surface. Simulations were performed on the lattice with 160×160 atom places for cyclic boundary conditions [1-2]. Surface step density oscillations along with a computer film demonstrating surface relief evolution during the growth process were obtained by simulation. Simulations of MBE growth processes on the vicinal surfaces with equidistant steps and echelons of steps as well as on the surfaces with initially formed two-dimensional islands at different effective surface temperatures were carried out. Surface step density oscillations of islands and steps in simulation process were compared with RHEED oscillations obtained during MBE growth of Ge on Ge(111) [3]. The lowest temperature of the surface corresponds to the three-dimensional growth mode and the highest one to step-flow mode.

Fig. 1(a) demonstrates RHEED oscillations obtained during homoepitaxy of Ge on the surface with (111) orientation at various surface temperatures and the deposition rate equal to 2.5 nm/min. Step density as a function of deposited dose is represented in Fig. 1(b). Migration length was measure of the effective surface temperature. In our model migration length is defined by the number of diffusion steps per unit time. Increasing of the surface temperature is equivalent to a rise in diffusion step numbers that is increasing diffusion length. The maximum migration length used in simulations corresponds to the pure step flow mode and the minimum one to the two-dimensional island growth mode. Three-dimensional growth mode was not considered in this work.

All results presented in Fig. 1(b) were obtained by simulation on the stepped surfaces. Maximum terrace width L was 160 atomic units. Terraces could be separated by monoatomic steps, or by steps echelons of four monolayers height. Oscillations damping shapes were depended on the parameter L/l. Three bottom curves Fig. 1(b) correspond to echelon type initial relief. For curves 1–2 parameter $L/l \gg 1$, so there were no step flow and no decay of echelons. Increasing number of the simulated curve corresponds to the increasing of L/l. For the curve number 1 L/l is so high that oscillations behavior
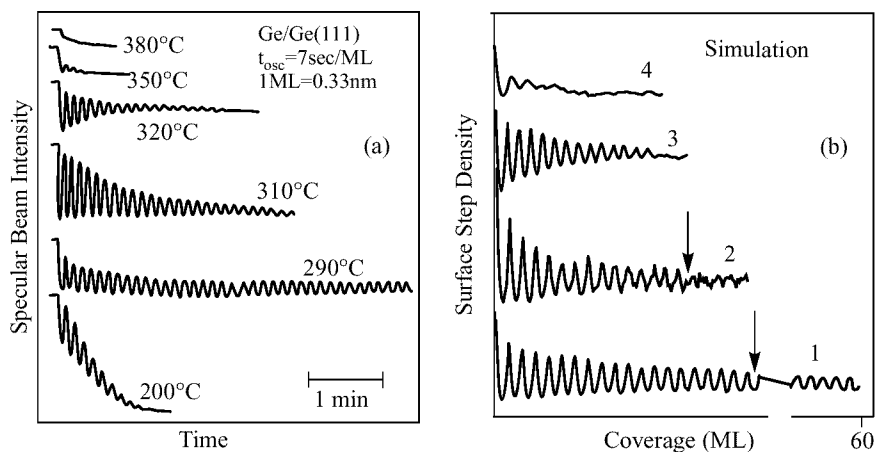
Fig 1.

is similar to their behavior on the flat surface. For the curve 2 echelons are practically undecayed during growth process but one could observe shift of the lower step in parallel with creation behind it of the region depleted with islands. This causes rapid damping of oscillations through forming specific structure of island with asynchronous nucleation [4]. Increasing of L/l brings to echelons decay: appearance of narrow terraces free of islands with simultaneous decrease of the initial terrace width with two-dimensional growth taking place. This fact causes rise of the lower envelope of the oscillation curve through surface step density decrease (curve 3 Fig. 1(b)). Further increase of L/l leads to complete decay of echelons and formation of the surface with equidistant steps. Initial relief with equidistant steps of monolayer height corresponds to curves 4 and 5. For migration length l of about $L/4$ one row of islands is continuously formed before moving step during growth process. One could see only one minimum in curve 4 during first monolayer deposition. No oscillation in step density curve could be seen for $L/l > 2$. Some decrease in step density with time appreciable in curve 5 could be associated with kinetic roughness of steps.

Surface relief formed due to coexisting of two growth modes during MBE process: two-dimensional island creation and step flow was considered. The reason of oscillations damping in chosen interval of parameters is not three-dimensional growth mode but creation of islands system reproducing in time named asynchronous structure [4]. The view of linear asynchronous structure is represented in Fig. 2(a). This type of surface relief corresponds to the curve 2 Fig. 1(b) after damping of oscillations. In this structure islands arranged along the lines parallel to the steps were nucleated simultaneously, however in given monolayer islands near the top terrace were nucleated earlier than others, and near the low one — later. Thus asynchronous nucleation took place. The moment of nucleation as well as the size of the island depend on the distance between the nucleus and the step. Linear asynchronous structure reproducing its form apparently moves during deposition process. So its perimeter in the average is remained constant causing damping of oscillations.

The top view of the surface corresponding to the curve 1 is represented in Fig. 1(b).
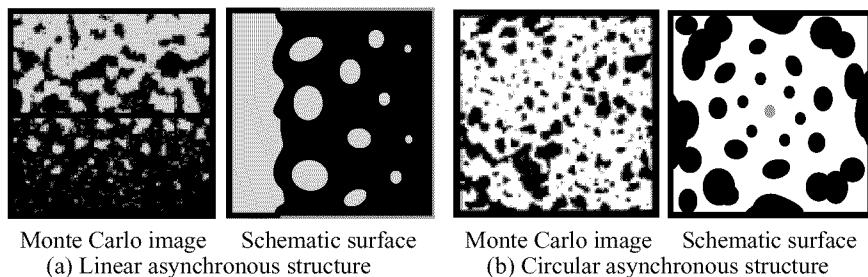
Monte Carlo image   Schematic surface   Monte Carlo image   Schematic surface
(a) Linear asynchronous structure   (b) Circular asynchronous structure

Fig 2.

The system of islands with increasing average radius as they move away from some center with vacancy-island could be seen in Fig. 1(b). Since islands near center with vacancy-island nucleated later than at the periphery due to the outflow of adatoms in vacancies such system of islands was named circular asynchronous structure. Circular asynchronous structure could be formed on the singular surfaces as well as on the vicinal ones with wide terraces without step flow. Oscillations damping in the initial part of the curve 1 Fig. 1(b) is accounted by the forming stage of circular asynchronous structure. Slightly damping oscillations observed late in time are characteristic of asynchronous structure of the circular form. Arrangement of such circular structures is maintained in every following monolayer.

One could often observe nonmonotonic amplitude modulations of RHEED oscillations in addition to their damping. Such type of distortions could be due to the initial relief which consists of steps of opposite directions and the coexistence of step flow and two-dimensional nucleation growth modes during growth process [5].

Simulation of MBE growth under changes of molecular beam intensity during deposition process demonstrates nonmonotonic amplitude distortions of step density oscillations mentioned above. This type of simulations was performed for explanation of available experimental RHEED oscillations obtained during Ge/Ge(111) deposition using two sources of different intensities [6]. Equivalent to variation of flux intensity in experiments is migration length variation according to the ratio $l \sim (D/I)^{(1/4)}$ [7] in simulations.
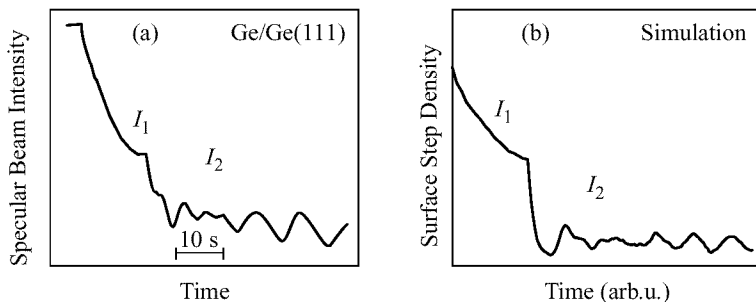

Fig 3.

RHEED oscillations and step density oscillations under changing flux intensity during

growth process are represented in Fig. 3. (I_1 — initial flux, I_2 — final flux, $I_1 < I_2$). For experimental and simulated curves one could observe similar oscillations shapes. After half monolayer deposition in low intensity flux large islands were formed on the terraces of simulated surface along with the creation of regions free of islands behind moving steps. Further deposition in higher flux results in simultaneous islands nucleation on the flat parts of the terraces and on the large islands grown earlier. Oscillation frequency of step density for these two systems of islands are different, that leads to the distortion of oscillations until the flux with intensity I_2 will determine growth process.

Thus the shape of RHEED oscillations is directly determined by the peculiarities of the surface morphology. Initial surface relief as well as its transformation during growth process influence on the oscillations shape. This allows in a number of cases just in the MBE process according to the shapes of oscillations to draw conclusions not only about the thickness of the layer but about its surface relief as well.

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